

INTRA AND INTERMOLECULAR DYNAMICS AND STRUCTURE IN THE FORMANILIDE-(H<sub>2</sub>O)<sub>n</sub> (n=1,2) CLUSTERS

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Formanilide (C<sub>7</sub>H<sub>7</sub>NO) is a molecule that mimics the -NH-CO- peptide bond. It adopts two different conformations, planar or non-planar, depending respectively on the *trans* or *cis* arrangement of the peptidic group. Formanilide offers a variety of hydrogen bond binding sites so its microsolvated clusters can be taken as good models to investigate the interaction of the peptide functional group with water. In this work, the rotational spectra of formanilide-(H<sub>2</sub>O)<sub>n</sub> (n=1, 2) complexes have been studied in the 2-12.5 GHz frequency range using both a pulsed-chirp and a molecular beam Fourier transform microwave spectrometers. Three heterodimers, *cis*-1:1a *trans*-1:1b and *trans*-1:1c forms and one heterotrimer, *cis*-1:2a, have been observed. The rotational spectra of the parent, several D/H and <sup>18</sup>O/<sup>16</sup>O isotopically substituted species have been measured for the adducts in order to investigate their structures. All species are characterized by the quadrupole coupling hyperfine structure due to the presence of a <sup>14</sup>N atom in formanilide. The rotational spectra of some species show small doublets attributable to either intramolecular motions within the formanilide subunit, as occur in *cis*-1:1a, or to intermolecular motions as the internal rotation of water in form *trans*-1:1c.